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6. AUTHORS
Richard Charnigo, Mathieu Francoeur, Cidambi Srinivasan

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
University of Kentucky
University of Kentucky Research Foundation
500 South Limestone Street
Lexington, KY 40526 -0001

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14. ABSTRACT
This transdisciplinary project sought to develop new statistical methods and theory for multivariate nonparametric regression along with a new analytic model for near-field emission by a nanoparticle on a surface. A short-term goal of the research was to establish a quantitative framework for characterizing nanoparticles nonintrusively and in real time on properties that could influence the near-field thermal spectrum in a nanoscale-gap thermophotovoltaic (nano-TPV) apparatus. A long-term goal was (and still is) to engineer nanostructured surfaces selectively emitting thermal radiation in the near field for efficient nano-TPV power generation. The short-term goal was pursued

15. SUBJECT TERMS
compound estimation, nanoparticle characterization, nano-thermophotovoltaic power generation, nonparametric regression, pattern recognition, scattering, Stein's phenomenon

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Report Title

FINAL REPORT FOR GRANT W911NF-12-1-0422

ABSTRACT

This transdisciplinary project sought to develop new statistical methods and theory for multivariate nonparametric regression along with a new analytic model for near-field emission by a nanoparticle on a surface. A short-term goal of the research was to establish a quantitative framework for characterizing nanoparticles nonintrusively and in real time on properties that could influence the near-field thermal spectrum in a nanoscale-gap thermophotovoltaic (nano-TPV) apparatus. A long-term goal was (and still is) to engineer nanostructured surfaces selectively emitting thermal radiation in the near field for efficient nano-TPV power generation. The short-term goal was pursued through three objectives: (1) develop theory and methods for compound estimation of mean response functions and their derivatives with multiple predictor variables and multiple outcome variables; (2) develop an analytic model for near-field thermal emission by a nanoparticle on a surface to describe how nanoparticle properties affect the near-field thermal spectrum; and, (3) assess the potential utility of a nanoparticle characterization framework based on the compound estimation of evanescent wave scattering patterns and their derivatives.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
10/20/2013	5.00	Sheila Edalatpour, Mathieu Francoeur. The Thermal Discrete Dipole Approximation (T-DDA) for near-field radiative heat transfer simulations in three-dimensional arbitrary geometries, Journal of Quantitative Spectroscopy and Radiative Transfer, (09 2013): 0. doi: 10.1016/j.jqsrt.2013.08.021
TOTAL:		**1**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Note: Papers related to these presentations have been and will be submitted for publication in peer-review journals, but the papers were not published as part of the proceedings for the conferences or invited presentations below. Abstracts for these presentations have been uploaded to the ARO extranet.

R. Charnigo and C. Srinivasan, “A multivariate generalized Cp and surface estimation,” University of Louisville, Louisville, KY, USA, November 15, 2013 (Invited presentation).

S. Edalatpour and M. Francoeur, “The Thermal Discrete Dipole Approximation (T-DDA) for numerical simulation of near-field thermal radiation,” ASME 2013 International Mechanical Engineering Congress & Exposition, San Diego, CA, USA, November 15-21, 2013.

S. Edalatpour and M. Francoeur, “The Thermal Discrete Dipole Approximation (T-DDA) for near-field radiative heat transfer calculations,” 2013 ASME Summer Heat Transfer Conference, Minneapolis, MN, USA, July 14-19, 2013.

S. Edalatpour and M. Francoeur, “Numerical simulation of near-field thermal radiation using the Thermal Discrete Dipole Approximation,” Electromagnetic and Light Scattering XIV, Lille, France, July 17-21, 2013.

L. Feng, R. Charnigo, and C. Srinivasan. “James-Stein type compound estimation of multiple mean response functions and their derivatives,” ENAR 2013 Spring Meeting, Orlando, Florida, USA, March 10-13, 2013.

M. Francoeur, “Design of thermal metamaterials beyond the effective medium theory: Direct numerical simulation via the Thermal Discrete Dipole Approximation (T-DDA),” Institut National des Sciences Appliquées (INSA) de Lyon, Villeurbanne, France, June 13, 2013 (Invited presentation).

M.R. Short, H. Tortel, A. Litman, J.-M. Geffrin, R. Vaillon, R. Abdeddaim and M. Francoeur, “Evanescent wave scattering by particles on a surface: Comparison between the discrete dipole approximation with surface interaction and the finite element method,” Electromagnetic and Light Scattering XIV, Lille, France, July 17-21, 2013.

Number of Presentations: 7.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
10/03/2013	1.00	Richard Charnigo, Limin Feng, Cidambi Srinivasan. Nonparametric and Semiparametric Compound Estimation in Multiple Covariates, Biometrics (06 2013)
10/03/2013	2.00	Richard Charnigo, Cidambi Srinivasan. A Multivariate Generalized C_p and Surface Estimation, Biostatistics (09 2013)
10/20/2013	6.00	Mitchell Short, Jean-Michel Geffrin, Rodolphe Vaillon, Herve Tortel, Bernard Lacroix, Mathieu Francoeur. Evanescent wave scattering by particles on a surface: Validation of the discrete dipole approximation with surface interaction against microwave analog experiments, Journal of Quantitative Spectroscopy and Radiative Transfer (10 2013)

TOTAL: **3**

Number of Manuscripts:

Books

Received	Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

No honors or awards were made specifically for any of the papers written under this ARO sponsorship. However, Dr. Charnigo was promoted from associate professor (with tenure) to full professor (with tenure) at the University of Kentucky, effective July 1, 2013, in part due to internal and external recognition of this ARO sponsorship. Moreover, Dr. Francoeur received the NSF Career Award in July 2013 for demonstrating experimentally enhanced power generation in nanoscale-gap thermophotovoltaic power generators; he believes that this ARO sponsorship contributed to his acquisition of the NSF Award.

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Limin Feng	0.08	
Sheila Edalatpour	0.11	
Mitchell Short	0.38	
FTE Equivalent:	**0.57**	
Total Number:	**3**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Richard Charnigo	0.12	
Cidambi Srinivasan	0.12	
Mathieu Francoeur	0.04	
FTE Equivalent:	**0.28**	
Total Number:	**3**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME	
Mitchell Short	
Total Number:	**1**

Names of personnel receiving PHDs

NAME	
Limin Feng	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

1 a. University of Utah

1 b. Office of Sponsored Projects
University of Utah
Salt Lake City UT 841128930

Sub Contractor Numbers (c): 304810995913116
Patent Clause Number (d-1): na
Patent Date (d-2): 8/15/12 12:00AM
Work Description (e): Develop a model for near-field thermal radiation calculations in complex three-dimensior
Sub Contract Award Date (f-1): 8/15/12 12:00AM
Sub Contract Est Completion Date(f-2): 7/31/13 12:00AM

1 a. University of Utah

1 b. Office of Sponsored Projects
1471 East Federal Way
Salt Lake City UT 841021821

Sub Contractor Numbers (c): 304810995913116
Patent Clause Number (d-1): na
Patent Date (d-2): 8/15/12 12:00AM
Work Description (e): Develop a model for near-field thermal radiation calculations in complex three-dimensior
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Sub Contract Est Completion Date(f-2): 7/31/13 12:00AM

Inventions (DD882)

Scientific Progress

Technology Transfer

FINAL REPORT FOR GRANT W911NF-12-1-0422

prepared by Richard Charnigo, Mathieu Francoeur, and Cidambi Srinivasan

**TABLE OF CONTENTS,
INCLUDING LISTS OF APPENDICES, ILLUSTRATIONS, AND TABLES**

Statement of the problem studied

This transdisciplinary project sought to develop new statistical methods and theory for multivariate nonparametric regression along with a new analytic model for near-field emission by a nanoparticle on a surface. A short-term goal of the research was to establish a quantitative framework for characterizing nanoparticles nonintrusively and in real time on properties that could influence the near-field thermal spectrum in a nanoscale-gap thermophotovoltaic (nano-TPV) apparatus. A long-term goal was (and still is) to engineer nanostructured surfaces selectively emitting thermal radiation in the near field for efficient nano-TPV power generation.

The short-term goal was pursued through three Objectives. The first Objective was to develop theory and methods for compound estimation of mean response functions and their derivatives with multiple predictor variables and multiple (possibly correlated) outcome variables. The second Objective was to develop an analytic model for near-field thermal emission by a nanoparticle (modeled as an electric point dipole) on a surface to describe how nanoparticle properties (e.g., size and refractive index) affected the near-field thermal spectrum. The third Objective entailed: (i) predicting the outcomes of laboratory experiments in which particles on a surface scattered evanescent waves generated by total internal reflection of an external radiation beam; and, (ii) assessing the potential utility of a nanoparticle characterization framework based on the compound estimation of evanescent wave scattering patterns and their derivatives.

Summary of the most important results

Our accomplishments are broadly summarized in the next three paragraphs, corresponding to the three Objectives from our proposal, and then described in further detail in the section below.

For Objective 1, the nonparametric regression technique of compound estimation was extended from the case of a single outcome variable and a single predictor variable [1] to scenarios with multiple predictor variables [2] and multiple outcome variables [3,4]. The former extension also allowed for some of the predictor variables to be handled nonparametrically while others were handled parametrically, an important consideration for problems in which the number of predictor variables is large and the curse of dimensionality is a concern [5]. The latter extension is remarkable in that nonlinear shrinkage a la Stein's phenomenon [6,7,8] can be exploited to reduce estimation error without sacrificing the self-consistency property that the estimated derivatives of the mean response function are in fact the derivatives of the estimated mean response function – a property not enjoyed by some widely accepted nonparametric regression techniques [9,10]. Besides the preceding, a new tuning parameter selection criterion called multivariate GC_p was developed to accommodate nonparametric regression models with multiple predictor variables whose realizations are irregularly distributed and in which the goal includes recovering derivatives of the mean response function rather than only the mean response function itself [11]. This criterion overcomes the limitations of numerous existing approaches, which are designed to work with only a single nonparametric regression technique [12,13], calibrated to recovery of the mean response function while not considering recovery of its derivatives [14,15], or confined to scenarios with a single predictor variable [16].

Regarding Objective 2, a novel method for solving near-field thermal radiation problems in complex three-dimensional geometries called the Thermal Discrete Dipole Approximation (T-DDA) has been developed, implemented and tested. The basics of the T-DDA and the validation of the approach have been published recently [17]. The T-DDA has been expanded to accommodate for interactions between arbitrarily-shaped objects of any size and a (semi-infinite) surface. The T-DDA with Surface Interaction (T-DDA-SI) has been verified against results for a nanoparticle, modeled as an electric point dipole, and a surface [18]. We are currently in the process of verifying the T-DDA-SI against experimental results for a large sphere (i.e., not modeled as an electric point dipole) and a surface [19]. A manuscript on the T-DDA-SI will be submitted in 2013 [20].

For Objective 3, predictions of evanescent wave scattering by particles on a surface have been performed using the Discrete Dipole Approximation with Surface Interaction (DDA-SI) [21,22]. For the first time, the DDA-SI has been validated using experimental data obtained from a scaled microwave apparatus [23,24]. Supplementary results from a finite element method (FEM) have been used for additional verifications. A good agreement between the DDA-SI and experimental data was found, thus suggesting that the DDA-SI can be employed as the forward model in an evanescent wave-based characterization framework. We now look forward to more fully developing the inverse model (i.e., creating and employing the statistical procedures that can convert experimental data on evanescent wave scattering into more accurate inferences about the particles' characteristics than is currently possible). Preliminary investigations using the compound estimation technique from Objective 1 have yielded mixed results but provide some cause for optimism [4]. Using an extensive database of simulated scattering data, we found that simultaneously using multiple outcome variables (corresponding to different elements of the Mueller scattering matrix [25]) for nanoparticle characterization yielded more accurate classifications than using a single outcome variable. Moreover, nonlinear shrinkage a la Stein's phenomenon [6,7,8] reduced the error in estimating scattering profiles and their derivatives. Yet, the reduced estimation error did not necessarily translate into more accurate classifications when these classifications were based on a principle of minimizing L^2 distance. Careful analysis of the results does, however, provide insights about what avenues to pursue next.

Details of scientific progress and accomplishments

Objective 1

Compound estimation was originally developed by Charnigo and Srinivasan [1] as a nonparametric regression technique for estimating the mean of a single outcome variable as a smooth function of a single predictor variable and, simultaneously, estimating the derivatives of the same function. Compound estimation possessed the self-consistency property that the derivatives of the estimated mean response function were exactly equal to the estimates of the derivatives. This property is not shared by the technique of local regression [9,10], which has been heralded for providing optimal convergence rates in nonparametric regression. Yet, Charnigo and Srinivasan [1] theoretically proved that compound estimation achieved virtually the same convergence rates, and they empirically demonstrated that compound estimation could substantially outperform local regression in finite samples. Thus, we were motivated to extend compound estimation to scenarios with multiple predictor variables [2] and multiple outcome variables [3,4].

Such scenarios have numerous practical applications. In addition to two biostatistical applications described later, another application of particular interest to our group is nanoparticle characterization. Here the multiple predictor variables could be observation angle and radiation wavelength, while the multiple outcome variables could convey multi-dimensional information about the manner in which nanoparticles to be characterized scattered evanescent waves; more specifically, the multiple outcome variables could correspond to distinct elements of the Mueller scattering matrix [25]. The idea is that nanoparticles of differing configurations should have their own characteristic mean response functions. Thus, upon acquiring scattering data from nanoparticles to be characterized, an experimenter could estimate the corresponding mean response functions and then "match" them (and their derivatives) to previously tabulated results in a "library" of mean response functions (and their derivatives) obtained from nanoparticles whose configurations were known. This idea was previously explored by our group [35,36,37] but only in scenarios with a single predictor variable and a single outcome variable (or, if there were multiple outcome variables, statistical inference for each one was treated in isolation from statistical inference for the others).

For the present research, then, we began by extending compound estimation to scenarios with multiple predictor variables [2]. As with a single predictor variable, differentiation and estimation were interchangeable in that the estimated derivatives of the mean response exactly equaled the corresponding derivatives of the estimated mean response. To illustrate this concept, Figure 1 in this final project report [2] depicts local regression estimates of a mean response and its first-order partial derivatives in proximity to a local minimum of the mean response, while Figure 2 [2] depicts compound estimates of the same. The estimates in Figure 1 conflict with each other, while those in Figure 2 are coherent: the estimated derivative of the mean response is the derivative of the estimated mean response. We theoretically proved that, in scenarios with multiple predictor variables, compound estimation achieved essentially optimal convergence rates for recovering the mean response and its partial derivatives. Moreover, as displayed in Table 1, compound estimation could reduce (a discrete approximation to mean integrated) squared error by amounts between 25% and 80% versus local regression.

We also explained how compound estimation could be employed even when some covariates were modeled parametrically and distinct observations on the same outcome variable might be correlated [2]. The former capability could be helpful for circumventing the curse of dimensionality [5] when there are numerous covariates but there is little reason to suspect that more than a couple of them have relationships with the outcome variable that need to be expressed nonparametrically. The latter capability could be valuable for repeated measures data. To illustrate, we applied compound estimation to a publicly available data set on telemonitoring in Parkinson's disease [38]. Taking into account the possible correlations among repeated measures on the same subject through random effects in a semiparametric regression model, we sought to relate the progression of Parkinson's disease (nonparametrically) to a subject's age and the signal fractal scaling exponent of the subject's recorded voice while adjusting (parametrically) for a number of other covariates. We discovered that, especially among those intermediate in age, an abnormal signal fractal scaling exponent might portend greater symptom progression. In addition, using compound estimation for inference on the nonparametric component of a semiparametric regression model might even reduce (versus local regression) Type II hypothesis testing errors on the parametric component.

We next extended compound estimation to multiple outcome variables [3,4]. An initial insight was obtained by writing out a local likelihood with multiple outcome variables and noting that the estimates for the mean response and its derivatives were invariant to the correlation (or lack thereof) between outcome variables. As such, handling the estimation for one outcome variable at a time is perhaps not as naïve as one may first suspect. However, while the correlation between outcome variables may not by itself call for a different estimation approach, the multiplicity of outcome variables may. We recalled Stein's phenomenon [6,7,8], which in effect says that the maximum likelihood estimator of a multivariate normal mean vector can be improved upon (in terms of expected squared error) through nonlinear shrinkage. In particular, every component of the maximum likelihood estimator should contribute to the estimation of any single component of the multivariate normal mean vector. Startlingly, this conclusion holds even when the covariance matrix is diagonal.

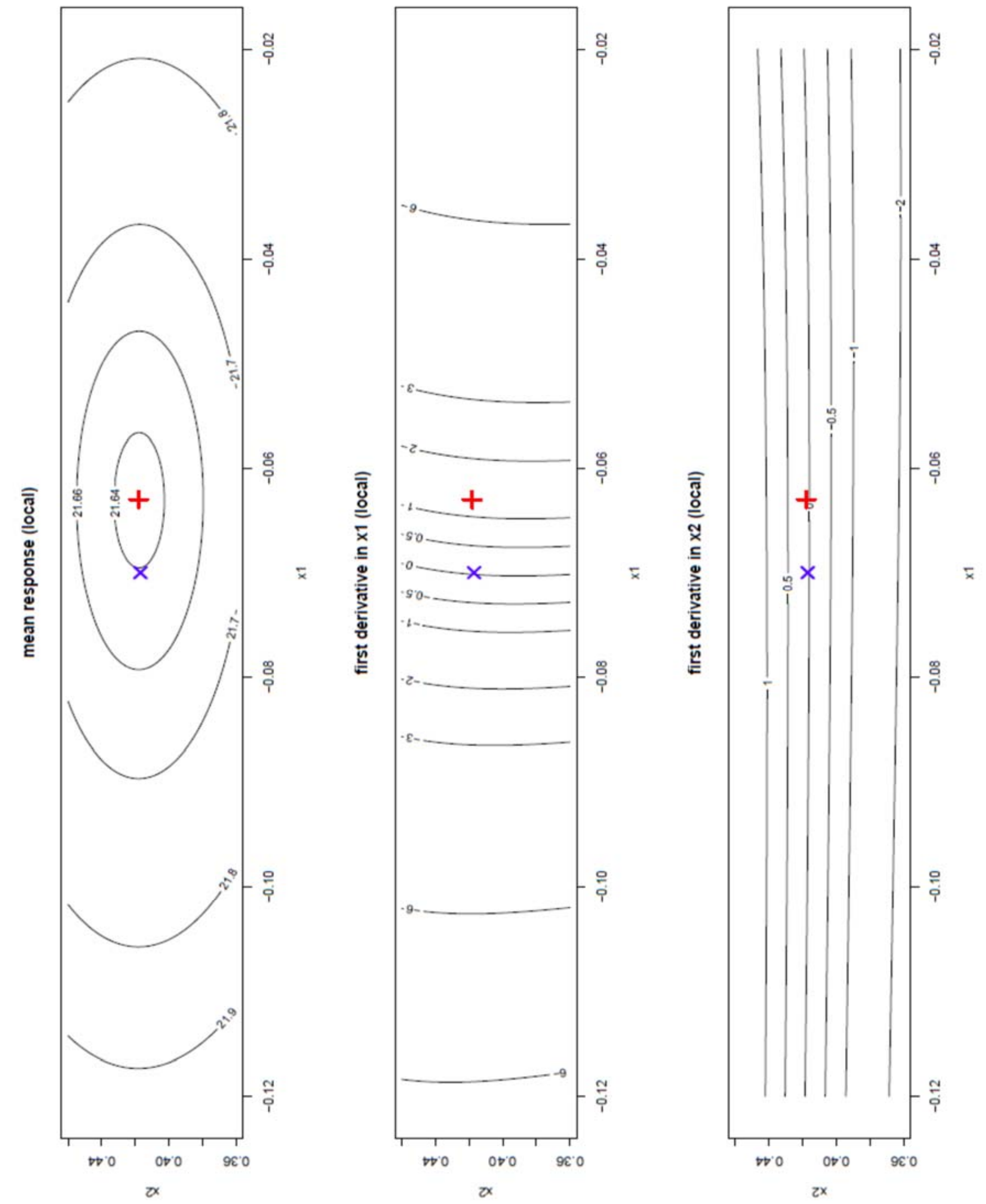


Figure 1 (adapted from [2]): Absence of self-consistency from local regression. The left panel depicts a close-up near a local minimum of a mean response function as inferred by local regression. The middle and right panels portray corresponding yet contradictory estimates of partial derivatives. In particular, the local minimum (marked by a + symbol) does not occur where both partial derivative estimates are zero (marked by a × symbol).

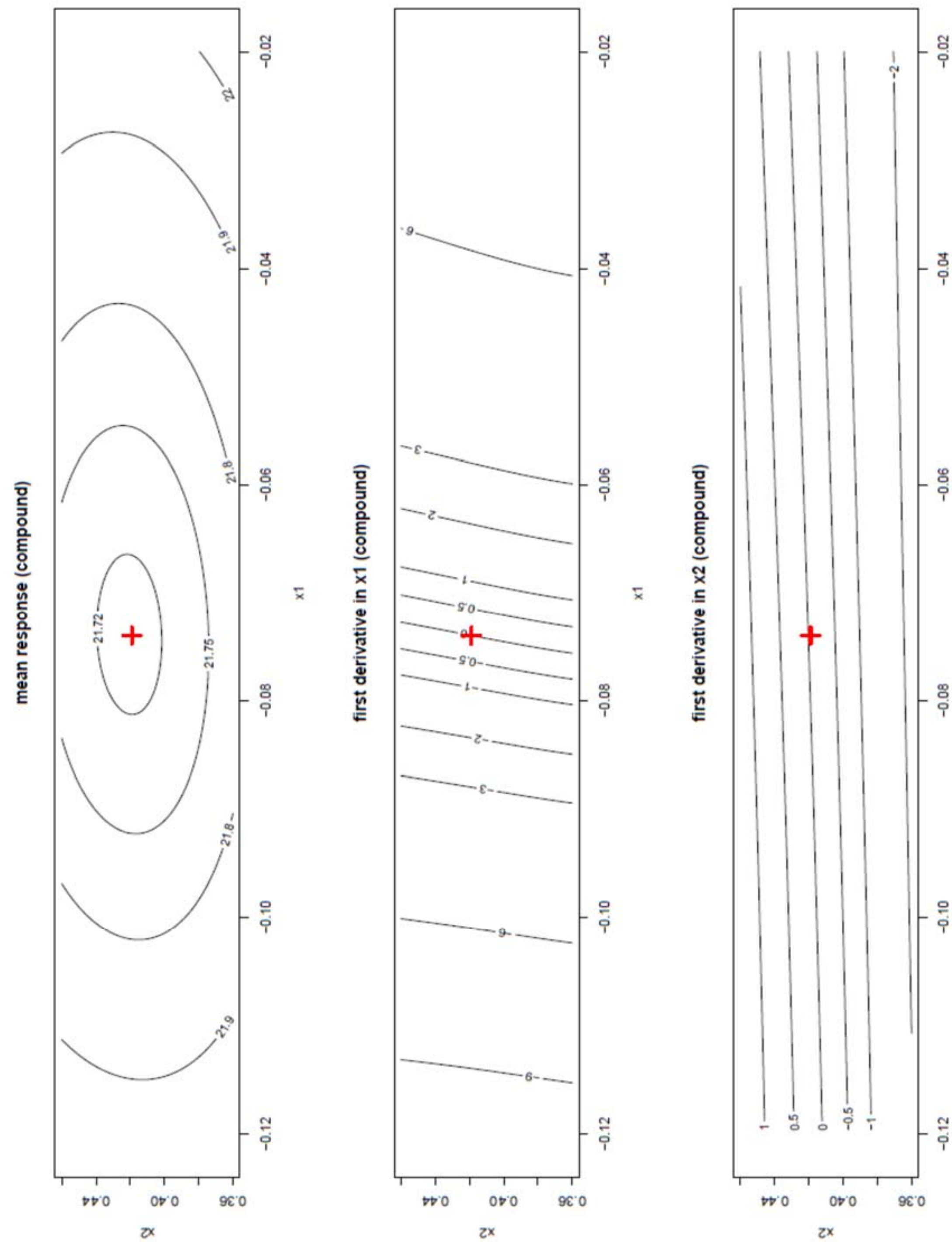


Figure 2 (adapted from [2]): Presence of self-consistency in compound estimation. The left panel depicts a close-up near a local minimum of a mean response function as inferred by compound estimation. The middle and right panels portray corresponding and compatible estimates of partial derivatives. In particular, the local minimum occurs precisely where both partial derivative estimates are zero (marked by a + symbol).

Target	Local regression, scenario 1	Compound estimation, scenario 1	Local regression, scenario 2	Compound estimation, scenario 2
mean response	42	31	40	29
first partial x_1	2,415	885	2,219	808
first partial x_2	2,534	934	2,363	819
mixed partial	16,824	12,236	15,939	11,988
second partial x_1	169,689	34,599	139,858	31,972
second partial x_2	181,616	44,768	157,398	33,621

Table 1 (adapted from [2]): Comparing compound estimation to local regression. Entries are the averages, over 100 simulated data sets, of the sums of squared errors in estimating the indicated targets via local regression and compound estimation. Both scenarios have $n = 225$, errors drawn from the standard normal distribution, and covariates regularly distributed on the unit square. Mean response function for scenario 1 is $\cos(3\pi x_1 / 2) + \sin(3\pi x_2 / 2)$, and mean response function for scenario 2 is $\arctan(2x_1) x_2^2 (6-x_2^2) / 2$.

Thus, we investigated how to incorporate Stein's phenomenon into nonparametric regression in the presence of multiple outcome variables, which may or may not be correlated [3,4]. The primary complication to extending the original results of Stein and James [6,7] turns out to be the bias inherent to nonparametric regression estimation. However, if one is willing to assume (or can estimate) an upper bound for the bias, then a similar nonlinear shrinkage – or "Steinization" – of nonparametric regression estimates can also be shown to reduce expected squared error [3]. Importantly, though perhaps not surprisingly, the magnitude of the shrinkage called for is related to this upper bound. In particular, large bias both calls for a lesser degree of shrinkage and portends fewer benefits from shrinkage. Thus, Steinization may be of most value in one of two situations: (i) tuning parameters are chosen that err on the side of "undersmoothing" the data; or, (ii) focus is on estimating the derivatives rather than (only) the mean response, since for given tuning parameters the bias/variance tradeoff tilts more toward variance as one differentiates. Of course, since our research agenda is particularly concerned with derivative estimation, finding (ii) is not unwelcome.

Figure 3 illustrates Steinization in nonparametric regression [4]. More specifically, local regression estimates of four different mean response functions are shown at each of 27 locations. In addition, local regression estimates of the derivatives of up to third order are acquired but are not depicted in Figure 3 to avoid making the graph illegible. Then Steinization is performed on a 16-dimensional object at each of the 27 locations, namely the vector whose components are the four mean response functions and their derivatives of up to third order at that location. One could similarly employ Steinization with compound estimation instead of local regression, but doing so would destroy the self-consistency property that motivated compound estimation in the first place. Thus, exploiting Stein's phenomenon in compound estimation is more delicate. One way to do so, and in fact what is actually shown in Figure 3, is to Steinize the pointwise estimates (acquired from local regression) that will be used in the first stage of compound estimation [1]. Then proceed with the second stage of compound estimation, namely the convolution of local polynomials defined using the pointwise estimates, in the manner previously advocated [1]. Since self-consistency is wholly a by-product of the convolution of local polynomials and has nothing to do with the properties of the pointwise estimates, self-consistency is not jeopardized. Yet, if the pointwise estimates are improved by Steinization, then one anticipates that the resulting compound estimates will likewise be improved.

What is described above is not the only way to exploit Stein's phenomenon in compound estimation. For instance, instead of performing Steinization on a 16-dimensional object at each of the 27 locations, Steinization could be performed on various nine-dimensional objects. One such object would be the estimates of the first mean response function at the first nine locations. Taking into account that there are three clusters of nine locations, four mean response functions, and derivatives of up to third order, one sees that there are 48 nine-dimensional objects on which Steinization could be performed. We refer to the former approach as "Steinization across outcomes and orders of derivatives" and to the latter as "Steinization across centering points". Simulation studies suggest that the latter approach may be more effective in reducing squared error and, not surprisingly given consideration (ii), that the benefits of Steinization are greater for estimating derivatives than for estimating mean responses [4]; see Table 2.

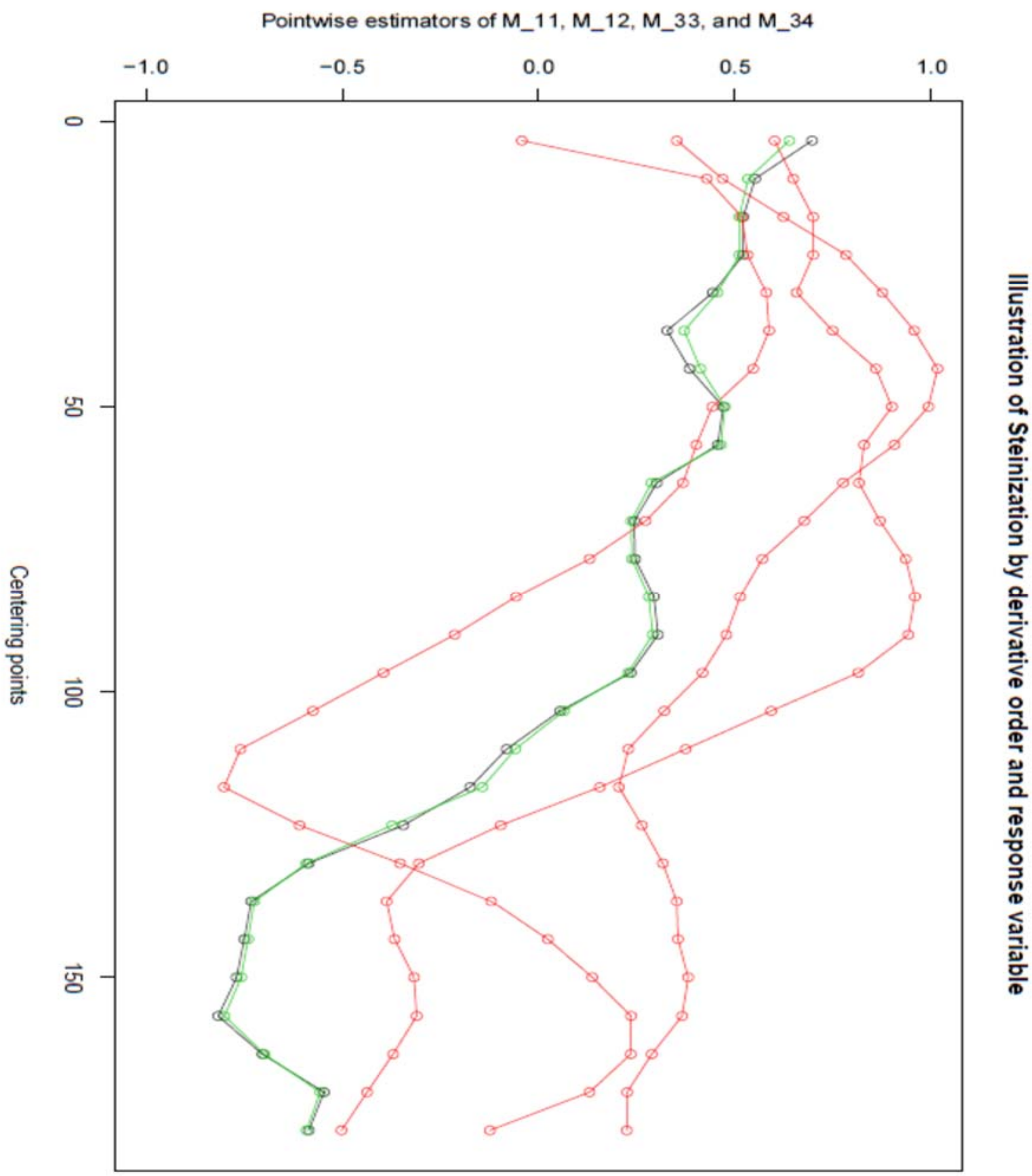


Figure 3 (adapted from [4]): Incorporating Steinization into nonparametric regression. Shown in black are pointwise estimates of an M_{34} scattering profile at the 27 centering points used in compound estimation, which are converted to the pointwise estimates in green after Steinization. Shown in red are pointwise estimates of M_{11}, M_{12}, and M_{33} scattering profiles. Pointwise estimates in green represent a compromise of pointwise estimates in black with pointwise estimates in red (along with 12 other sets of pointwise estimates not displayed to avoid making the graph illegible), which is most easily seen at the top of the graph.

Squared error of estimation for:	Scenario 1 w/ and w/o Steinization	Scenario 2 w/ and w/o Steinization	Scenario 3 w/ and w/o Steinization	Scenario 4 w/ and w/o Steinization
mean responses	0.255; 0.273 (7% reduction)	0.125; 0.126 (1% reduction)	0.269; 0.272 (1% reduction)	0.125; 0.125 (0% reduction)
first derivatives	0.151; 0.202 (25% reduction)	0.049; 0.056 (13% reduction)	0.200; 0.205 (2% reduction)	0.055; 0.055 (0% reduction)
second derivatives	0.135; 0.196 (31% reduction)	0.042; 0.051 (18% reduction)	0.196; 0.200 (2% reduction)	0.050; 0.050 (0% reduction)
summation	0.541; 0.671 (19% reduction)	0.216; 0.233 (7% reduction)	0.665; 0.677 (2% reduction)	0.229; 0.230 (0% reduction)

Table 2 (adapted from [4]): Effects of Steinization on estimation error. Entries are averages, over 600 data sets designed to mimic results from scattering experiments intended for nanoparticle characterization [37], of the sum of squared errors in estimating four mean response functions (corresponding to four distinct elements of the Mueller scattering matrix [25]), their first derivatives, and their second derivatives, expressed as fractions of the squared Frobenius norm of the nonparametric regression smoothing matrix in the absence of Steinization. **Scenarios 1 and 2** entailed compound estimation with Steinization of local regression pointwise estimates across clusters of nine centering points, while **Scenarios 3 and 4** entailed compound estimation with Steinization of local regression pointwise estimates across four outcome variables and orders of derivatives. Scenarios 1 and 3 had a signal to noise ratio of 4, while Scenarios 2 and 4 had a signal to noise ratio of 16. The shrinkage factors used in Steinization assumed that estimation bias in nonparametric regression was negligible relative to estimation variance.

Our final endeavor for Objective 1 was to develop a tuning parameter selection criterion for nonparametric regression problems with multiple covariates whose values may be irregularly spaced, when there is interest in estimating derivatives of a mean response function rather than (only) the mean response function itself [11]. Apart from an asymptotically negligible remainder, our multivariate generalized C_p (GC_p) has expected value equal to the sum of squared errors of a fitted derivative, which cannot be calculated in practice because the true derivative is unknown. Thus, multivariate GC_p is a data-based proxy for this sum of squared errors whose minimization is hoped to also (approximately) minimize the sum of squared errors.

The statistical motivation for developing multivariate GC_p is that existing tuning parameter selection criteria have (at least) one of the following limitations:

(i) They may minimize a proxy for the sum of squared errors of the fitted mean response function, not the fitted derivative, potentially leading to undersmoothed estimated derivatives [14,15].

(ii) They may be designed to work with a single nonparametric regression method, such as local regression [12] or spline smoothing [13], without being applicable to other nonparametric regression methods.

(iii) They may only accommodate scenarios with one predictor variable [16].

However, multivariate GC_p does not have these limitations. In fact, multivariate GC_p can be used with any nonparametric regression method that produces estimates linear in the outcome variable at particular values of the tuning parameters.

Besides the potential application in nanoparticle characterization, a motivating biostatistical application that we pursued was to relate a person's blood level of bilirubin (one measure of liver function) to the two principal components defined by his or her levels of aspartate aminotransferase (AST) and alanine aminotransferase (ALT) (two other measures of liver function, which may be easier and less expensive to monitor routinely [39]). Using publicly available data [40], we compared multivariate GC_p to ordinary C_p and generalized cross validation [14,15] (among other tuning parameter selection methods) in their abilities to recover good tuning parameters for compound estimation [2] of the aforementioned relationship.

Figure 4 displays the estimated mean responses, while Figure 5 displays the estimated partial derivatives with respect to the first principal component. The latter graph is particularly revealing because negative fitted values occur when ordinary C_p and generalized cross validation select tuning parameters. Moreover, these negative fitted values are difficult to defend because they occur in a region where the data are sparse. In contrast, no such artifacts are observed when multivariate GC_p selects tuning parameters. And, unlike the estimate resulting from ordinary C_p and generalized cross validation, this estimate does not appear to be undersmoothed. In fact, a simulation study suggests that multivariate GC_p leads to more accurate estimation of first-order derivatives than ordinary C_p and generalized cross validation, at least when the signal to noise ratio is not too low; see Table 3. When the signal to noise ratio is very low, conventional tuning parameter selectors may fare comparatively well because their tendencies to undersmooth are negated by very high noise. However, in such cases, one may question the appropriateness of attempting to estimate derivatives at all.

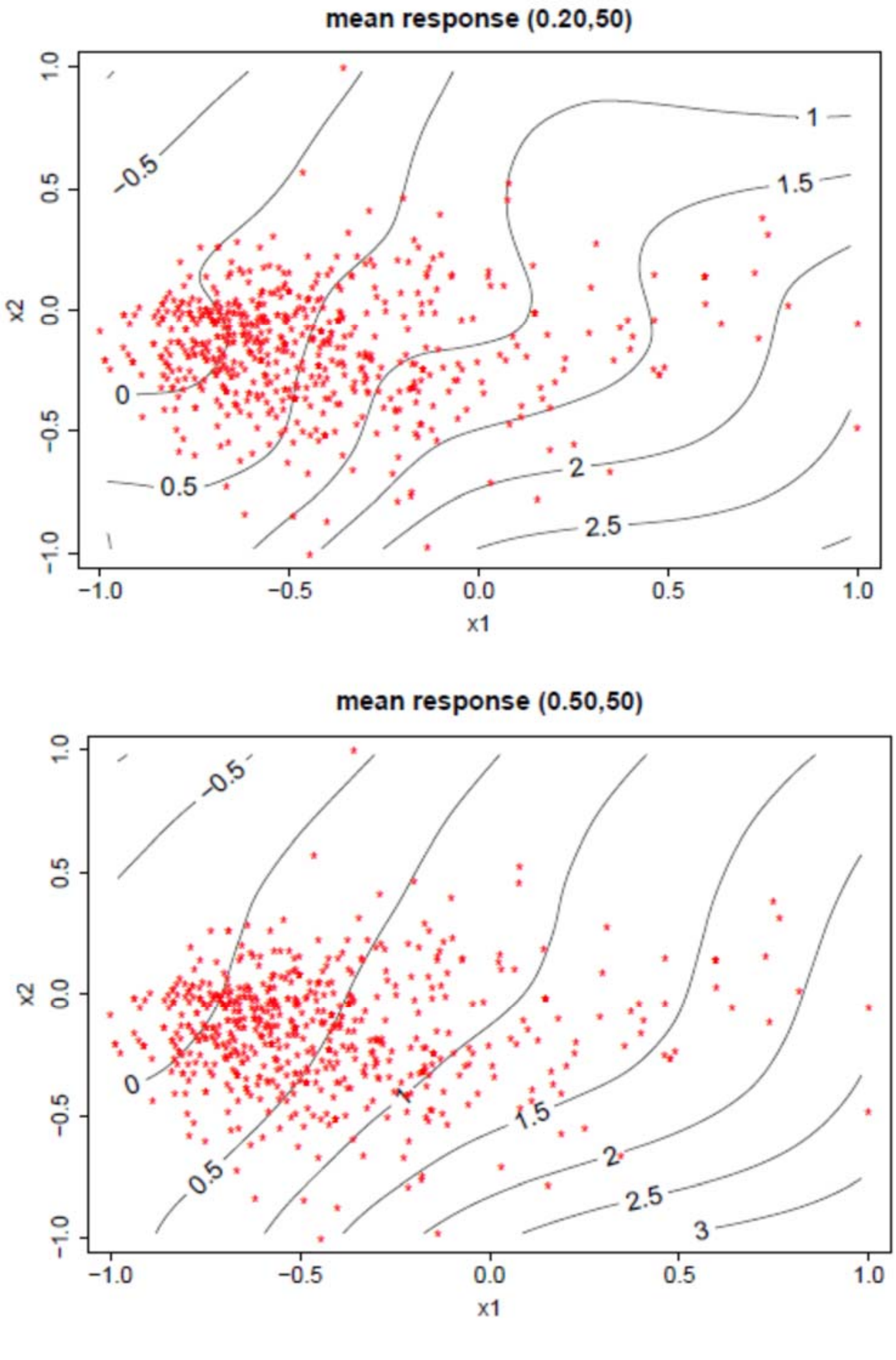


Figure 4 (adapted from [11]): Tuning parameter selection and mean response estimation. Displayed are two compound estimates of a mean response function. For the top estimate, tuning parameters (0.20 nearest neighbor fraction and 50 convolution parameter) were selected by C_p and generalized cross validation. For the bottom estimate, tuning parameters (0.50 and 50) were selected by multivariate GC_p. Superimposed in small * symbols are the predictor variable values.

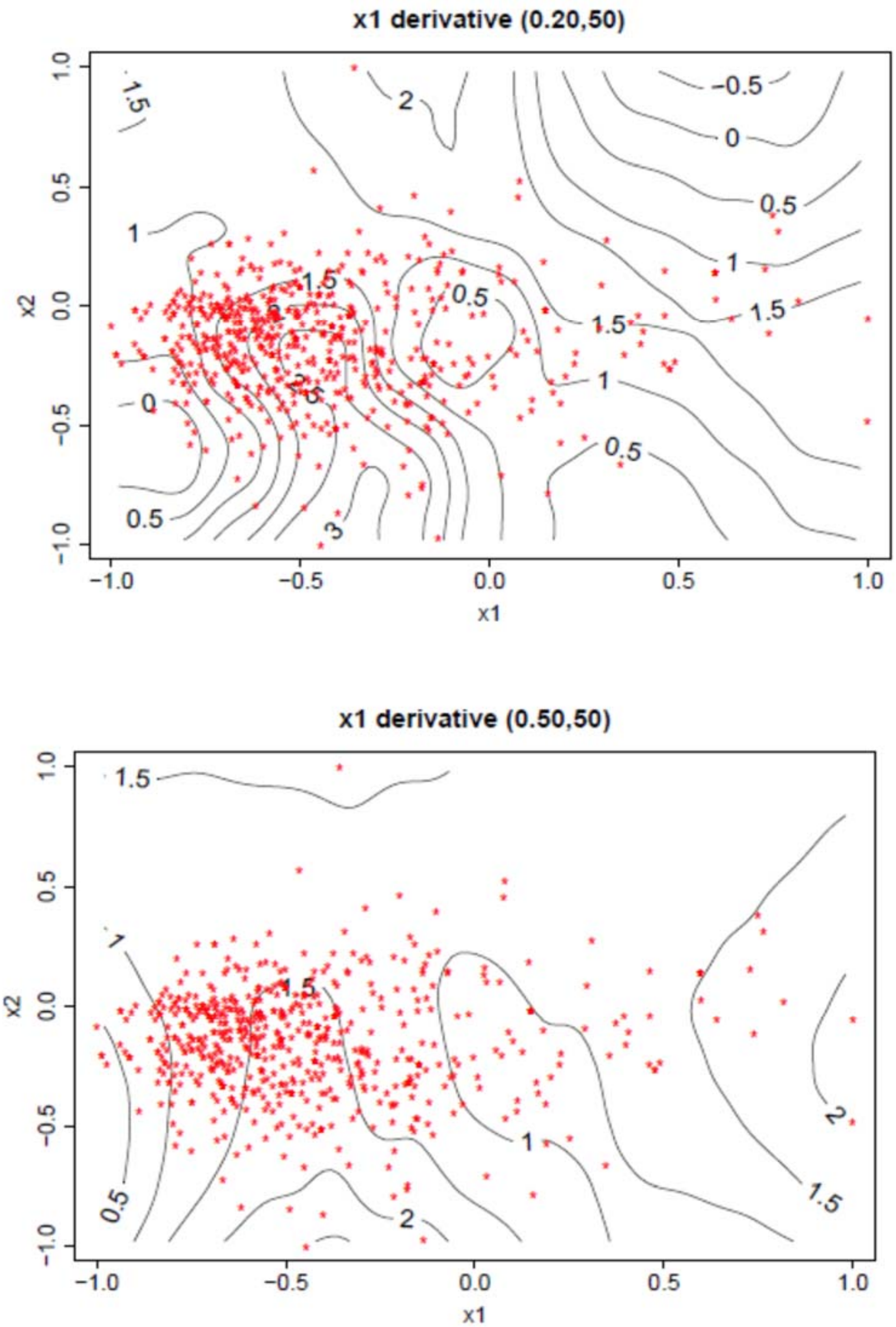


Figure 5 (adapted from [11]): Tuning parameter selection and partial derivative estimation. Displayed are two compound estimates of a first-order partial derivative of a mean response function. For the top estimate, tuning parameters (0.20 nearest neighbor fraction and 50 convolution parameter) were selected by C_p and generalized cross validation. For the bottom estimate, tuning parameters (0.50 and 50) were selected by multivariate GC_p. Superimposed in small * symbols are the predictor variable values.

Scenario	multivariate generalized C_p	ordinary C_p	generalized cross validation
1	1.07	1.08	1.08
2	1.10	1.14	1.14
3	1.14	1.10	1.10
4	1.07	1.13	1.13
5	1.07	1.08	1.08
6	1.07	1.05	1.05

Table 3 (adapted from [11]): Comparing multivariate generalized C_p to its competitors. Each entry is the median over 100 simulated data sets of the ratio of the squared error in estimating first-order derivatives achieved with the tuning parameter selection criterion divided by the smallest possible squared error that could be achieved by an oracle selecting the best tuning parameters. The mean response function in scenarios 1, 2, and 3 is defined to be the graph in the top panel of Figure 4, while the mean response function in scenarios 4, 5, and 6 is defined to be the graph in the bottom panel. For scenarios 1 and 4, error variances were two-thirds the magnitude estimated from the original data set; for scenarios 2 and 5, equal to that magnitude; for scenarios 3 and 6, three-halves that magnitude.

Objective 2

Edalatpour and Francoeur [17] developed a novel framework for solving near-field thermal radiation problems in three-dimensional arbitrary geometries. The method called the T-DDA does not make any assumptions on the shape and the size of the objects as well as on their separation distances. In the T-DDA, objects are discretized into cubical sub-volumes conceptualized as electric point dipoles. After discretization, the following system of equations is obtained:

$$\overline{\overline{\mathbf{A}}} \cdot \overline{\mathbf{P}} = \overline{\mathbf{E}}_{inc} \tag{1}$$

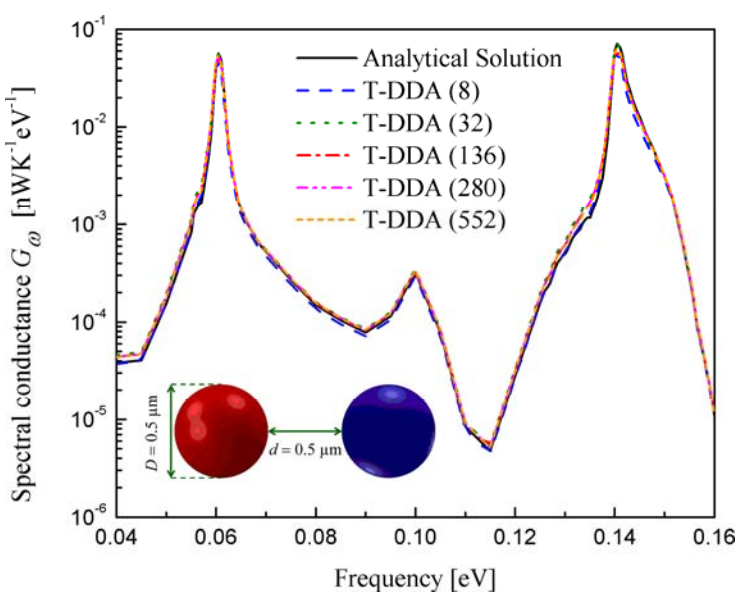
where $\overline{\overline{\mathbf{A}}}$ is the 3N by 3N interaction matrix (N is the number of sub-volumes), $\overline{\mathbf{E}}_{inc}$ is the 3N column vector containing the incident field and $\overline{\mathbf{P}}$ is the 3N column vector containing the unknown dipole moments. The form of Eq. (1) is the same as the system of equations employed in regular DDA methods for predicting light scattering by particles [26]. However, in thermal radiation problems, the incident field is due to thermal emission, such that $\overline{\mathbf{E}}_{inc}$ is a stochastic vector. Consequently, the unknown dipole moment vector $\overline{\mathbf{P}}$ is also stochastic.

The first moment (mean) of the incident field is zero, while its second moment is computed via the fluctuation-dissipation theorem (FDT) [27]. The FDT relates thermal fluctuations of currents inside a body to its local temperature. The quantity of interest in radiation heat transfer is the net power exchanged that is proportional to the trace of the dipole auto-correlation function. This implies that the instantaneous dipole moment vector $\overline{\mathbf{P}}$ does not need to be calculated directly (only the auto-correlation function of $\overline{\mathbf{P}}$ is needed). This fact is extremely important, as it shows that the T-DDA is a deterministic method even if near-field thermal radiation problems are fundamentally stochastic.

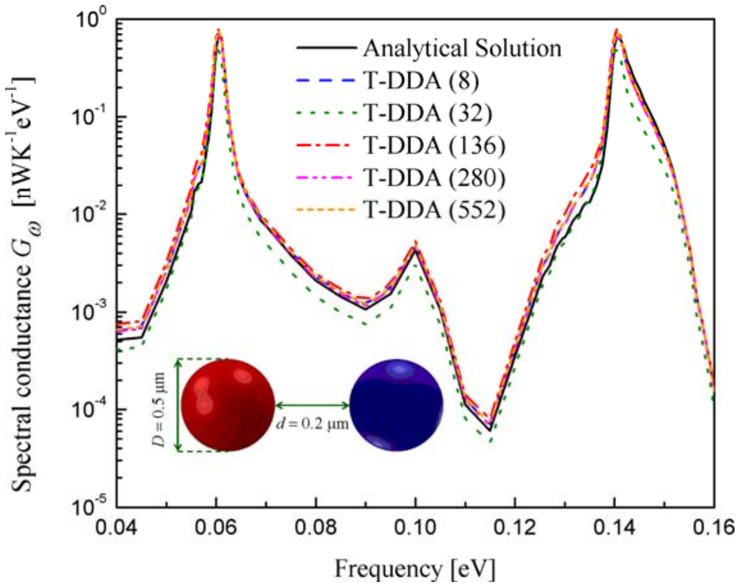
The T-DDA has been tested against the analytical solution of Narayanaswamy and Chen where near-field radiative heat transfer between two large spheres is calculated [28]. More specifically, the quantity reported is the thermal radiative conductance defined as follows:

$$G_\omega = \lim_{\delta T \to 0} \frac{\langle Q_{net,\omega} \rangle}{\delta T} \tag{2}$$

where $Q_{net,\omega}$ is the net heat rate between the objects while T is the temperature. Figure 6 shows the conductance for two spheres made of silica calculated using the T-DDA and the analytical solution of Narayanaswamy and Chen. The diameters of the spheres are fixed at 0.5 μm while the temperature is kept at 400 K; separation distances of 0.5 and 0.2 μm are considered in panels (a) and (b), respectively.



(a)



(b)

Figure 6. Spectral conductance between two silica spheres for separation gaps of: (a) 0.5 μm, and (b) 0.2 μm (the numbers in parentheses correspond to the number of sub-volumes in each sphere).

It can be seen that the T-DDA is in excellent agreement with the analytical solution. For 552 sub-volumes in each sphere, the relative differences between the total conductance (i.e., integrated over all frequencies) calculated from the T-DDA and the analytical solution are 0.35% and 6.4% for separation gaps of 0.5 and 0.2 μm, respectively.

The analytical solution of Narayanaswamy and Chen [28] is based on a complicated and cumbersome expansion of the fields in vector spherical harmonics (Mie-type solution), and is thus restricted to the two-sphere configuration. For instance, the case of three spheres cannot be treated with the solution of Ref. [28], while it is straightforward to add objects in the T-DDA. Additionally, the T-DDA is versatile as any type of geometries can be considered. As an illustrative example, the conductance between two cubes of silica calculated with the T-DDA is shown in Figure 7. Both cubes have side length of 0.5 μm and are separated by a distance of 0.5 μm; as before, the temperature is fixed at 400 K. Note that an analytical solution does not exist for this problem.

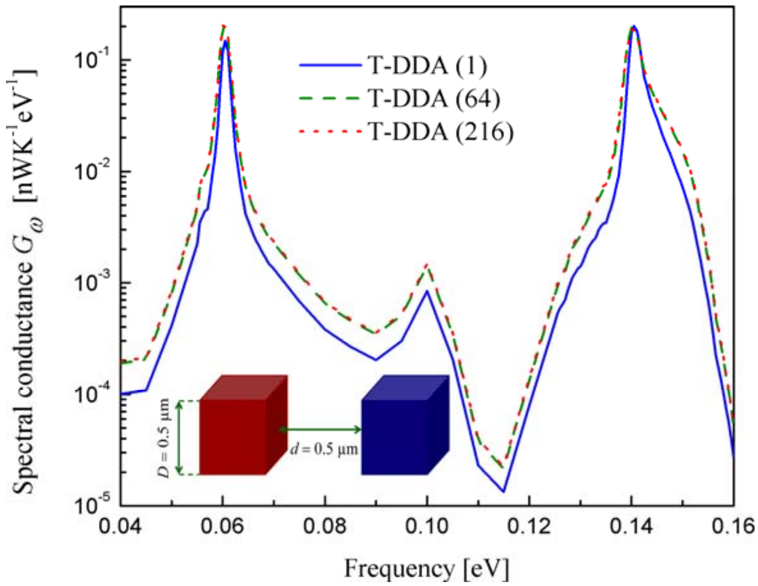


Figure 7. Spectral conductance between two silica cubes separated by a 0.5 μm-thick gap (the numbers in parentheses correspond to the number of sub-volumes in each cube).

A fast convergence of the T-DDA is observed in Figure 7. The relative difference between the total conductance for 64 and 216 sub-volumes in each cube is 1.5%, while the relative difference is 0.6% between 216 and 512 sub-volumes (result not shown).

A further development of the T-DDA is the addition of a semi-infinite surface (method called T-DDA-SI). No such model currently exists in the literature. This allows for the very first time to account for the interactions between objects of arbitrary shapes and sizes and a surface. The T-DDA-SI will impact not only nano-TPV power generation, but also applications such as thermal microscopy [29].

The presence of the surface modifies the original T-DDA formulation in two ways [30,31]. First, the incident should account for waves emitted by dipoles that reflect off the surface before reaching another dipole. Secondly, the interaction mechanism between dipoles *i* and *j* is modified by adding an extraneous contribution due to radiation from dipole *j* that reflects off the surface before reaching dipole *i*. In the presence of a surface, the linear system of equations to be solved becomes:

$$\left(\overline{\overline{\mathbf{A}}} + \overline{\overline{\mathbf{R}}}\right) \cdot \overline{\mathbf{P}} = \overline{\mathbf{E}}_{inc} \tag{3}$$

where $\overline{\overline{\mathbf{R}}}$ is the deterministic reflection-interaction matrix. The integration of surface interactions within the T-DDA is essentially based on the work of Sommerfeld that analyzed electric dipole radiation above a semi-infinite plane [32]. The electric field reflected off the surface is calculated using the Sommerfeld identity [33]:

$$\frac{e^{ik_0 r}}{4\pi r} = \frac{i}{4\pi}\int_0^\infty \frac{k_\rho}{k_{z0}} J_0(k_\rho \rho) e^{ik_{z0}|z|}\, dk_\rho \tag{4}$$

where k_ρ and k_{z0} are respectively the wavevectors parallel and perpendicular to the surface, while J_0 is the Bessel function of the zeroth order. The purpose of the Sommerfeld identity is to decompose spherical waves into a summation of cylindrical waves propagating parallel to the surface and plane waves propagating along the *z*-direction normal to the surface. As such, the cylindrical waves do not interact with the surface; only the plane waves interact with the surface, and this interaction is calculated via the standard Fresnel reflection coefficients.

By performing this analysis for the horizontal electric dipole and the vertical electric dipole oscillations (relative to the surface), the electric fields reflected off the surface in both TM and TE polarizations due to dipole radiation are calculated. These reflected electric fields are then added to the incident field vector $\overline{\mathbf{E}}_{inc}$. The reflected electric fields are also employed for populating the reflection-interaction matrix. This is done by considering the reflected field at $\mathbf{r}_i$ due to dipole radiation at $\mathbf{r}_j$:

$$\mathbf{E}_{ref,i} = \overline{\overline{\mathbf{R}}}_{ij} \cdot \mathbf{p}_j \tag{5}$$

Using the reflected electric fields in combination with Eq. (5), the expression for the local reflection-interaction matrix $\overline{\overline{\mathbf{R}}}_{ij}$ for all dipole pairs is derived. Then, the global reflection-interaction matrix $\overline{\overline{\mathbf{R}}}$ can be populated. The mathematical details are omitted here due to lengthy equations. With the T-DDA-SI, near-field thermal radiation problems in three-dimensional complex geometries involving objects near or on a surface are tractable for the very first time. It is worth noting that the extension to multiple surfaces is straightforward via calculation of plane wave reflection and transmission from multiple plane layers [31].

Figure 8 shows a proof-of-concept of the T-DDA-SI, where the net heat transfer between a nanoparticle at 300 K (radius of 1 μm; modeled as a single electric point dipole) and a surface at 321 K, both made of silica, is shown as a function of the gap. Note that the gap here corresponds to the distance between the edge of the particle and the surface.

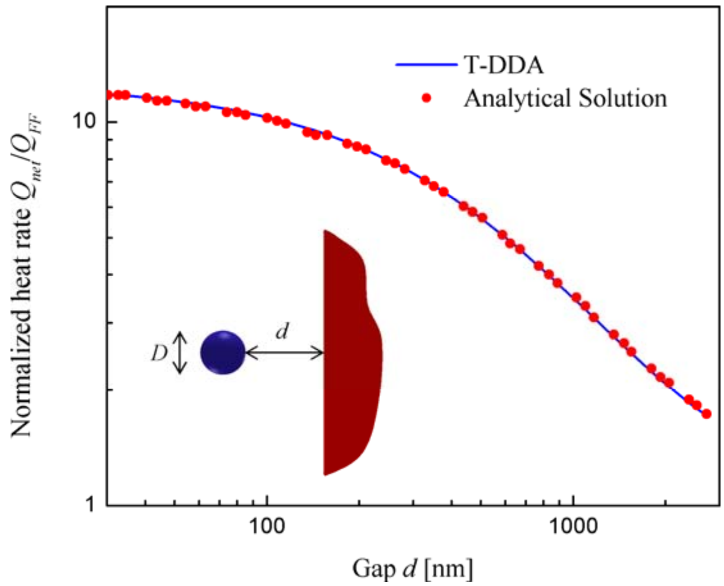


Figure 8. Net heat transfer (normalized by the far-field heat transfer) between a dipole and a surface: Comparison between T-DDA-SI and Otey and Fan [18].

Results from the T-DDA-SI are in perfect agreement with those from Otey and Fan [18] for a nanoparticle exchanging radiation with a surface. The T-DDA-SI is currently being validated against experimental data for a large sphere and a surface [19]. These results along with the details of the T-DDA-SI will be discussed in a paper to be submitted in 2013 [20].

Objective 3

The evanescent wave-based characterization framework includes three essential components: (1) the forward model for predicting evanescent wave scattering by particles on a surface, (2) an experimental device for measuring scattering profiles, and (3) an inversion algorithm in order to retrieve the nanoparticles' characteristics from measured scattering profiles. Prediction of evanescent wave scattering by particles on a surface is accomplished via the Discrete Dipole Approximation with Surface Interaction (DDA-SI) [21,22]. In this work, significant progresses have been made in the establishment of the DDA-SI as a forward model for the characterization framework.

In order to assess the accuracy of the forward model in the characterization framework, the DDA-SI has been validated for the first time against scaled microwave experimental results [23,24]. Multiple experiments were made in the frequency band of from 4 to 6 GHz (wavelengths λ of from 5 to 7.5 cm) for a variety of lossless and lossy cubes and spheres with size parameters of from $\lambda/2.5$ to $\lambda/0.83$. Figures 9 to 11 show selected validation results, where it is clear that the DDA-SI provides accurate predictions of evanescent wave scattering by particles on a surface. Note that results from a FEM are also included for supplementary verifications.

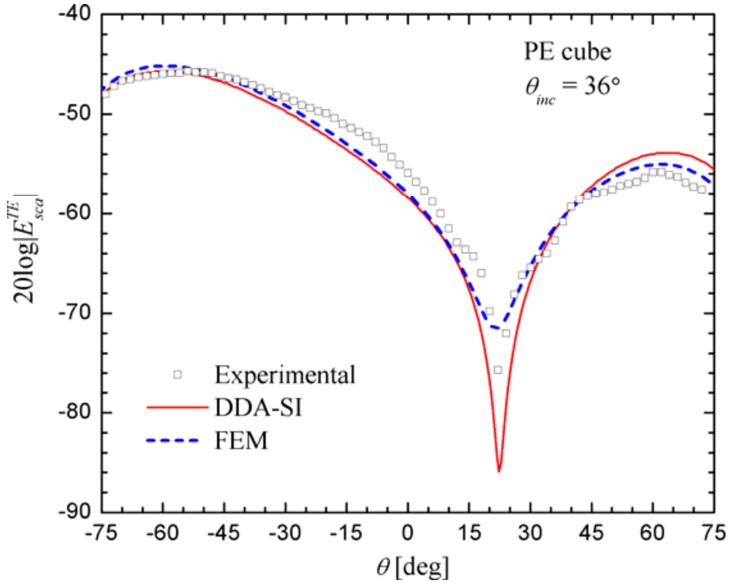


Figure 9. TE-polarized electric field scattered in the far zone by a lossless cube ($\lambda/1.785$ side length) illuminated by an evanescent wave: Comparison between experimental, DDA-SI and FEM results.

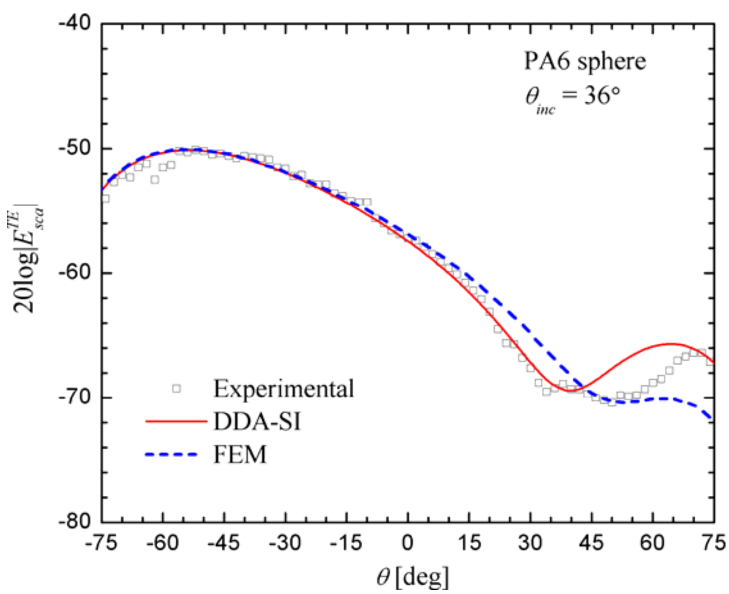
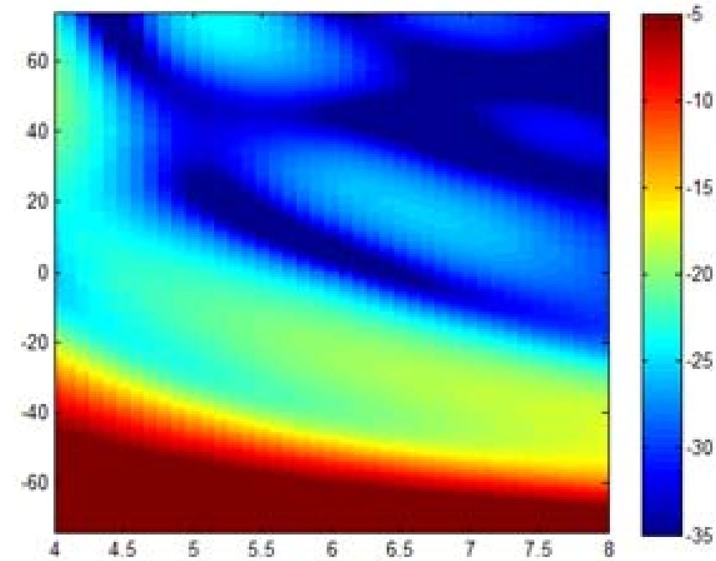


Figure 10. TE-polarized electric field scattered in the far zone by a lossless sphere ($\lambda/1.923$ diameter) illuminated by an evanescent wave: Comparison between experimental, DDA-SI and FEM results.



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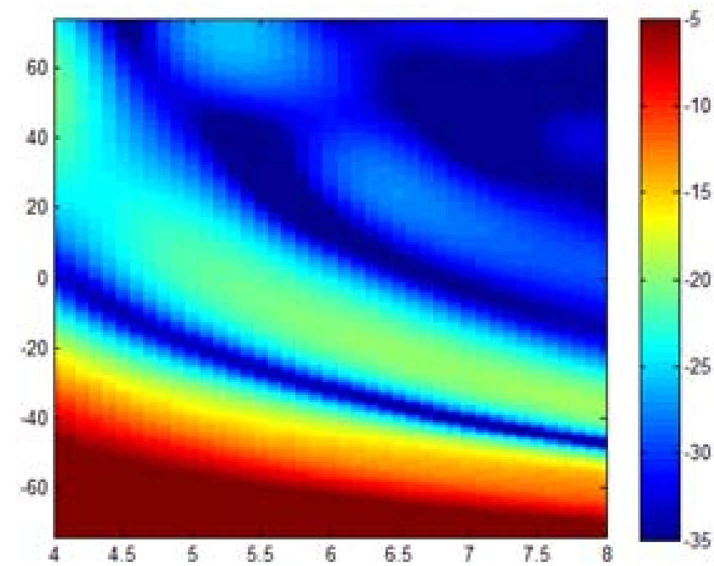
(a)



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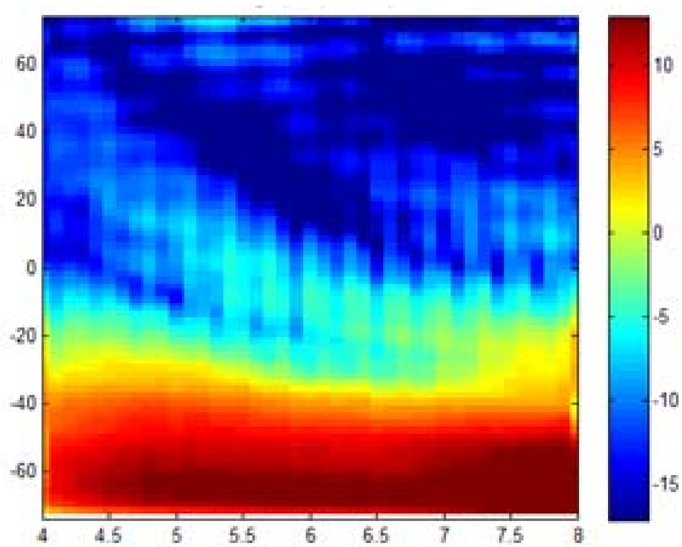
(b)



(c)

Figure 11. TE-polarized electric field scattered in the far zone by an absorbing sphere (λ/0.865 diameter) illuminated by an evanescent wave: (a) DDA-SI. (b) FEM. (c) Experimental results.

Additionally, an extensive sensitivity analysis of the Mueller matrix elements to the particles' properties has been conducted via the DDA-SI. The results of this sensitivity analysis, defining the best elements to employ in order to characterize a given parameter, are available in the MS thesis of Short [34].

The preceding suggests that the DDA-SI can be employed as the forward model in an evanescent wave-based characterization framework. Our future research agenda will include development of the corresponding inverse model. Preliminary investigations have already been undertaken to assess the viability of compound estimation for that purpose.

Recall from our description of progress for Objective 1 that compound estimation was adapted to multiple outcome variables [4] (corresponding to, for example, multiple elements of the Mueller scattering matrix [25]) by incorporating nonlinear shrinkage a la Stein's phenomenon [6,7,8]. So far we have considered two forms of Steinization for compound estimation, one in which local regression pointwise estimates in clusters of nine points are shrunk toward each other, and one in which local regression pointwise estimates in groups of sixteen (defined by four different outcome variables and orders of derivatives under consideration) are shrunk toward each other. As previously shown in Table 2, both forms of Steinization can reduce estimation error if the signal-to-noise ratio is not too high, and Steinization across centering points can do so even if the signal-to-noise ratio is rather high.

However, as Table 4 reveals, reduced estimation error does not necessarily translate into more accurate nanoparticle characterization. Such a disparity seems to occur because, while Steinization tends to reduce the L^2 distance between the scattering profiles estimated from a noisy data set to the actual scattering profiles for nanoparticles of the same configuration (and similarly for the respective derivatives), Steinization also tends to reduce the L^2 distance between the estimated scattering profiles and the actual scattering profiles for nanoparticles of different configurations (and, again, similarly for the respective derivatives).

Correct classification rates based on minimization of L^2 distance between:	Scenario 1 w/ and w/o Steinization	Scenario 2 w/ and w/o Steinization	Scenario 3 w/ and w/o Steinization	Scenario 4 w/ and w/o Steinization
mean responses	537/600; 541/600	552/600; 552/600	545/600; 546/600	552/600; 554/600
first derivatives	448/600; 440/600	550/600; 550/600	453/600; 453/600	544/600; 543/600
second derivatives	276/600; 263/600	379/600; 374/600	253/600; 253/600	352/600; 354/600
summation	543/600; 547/600	561/600; 563/600	551/600; 551/600	559/600; 559/600

Table 4 (adapted from [4]): Effects of Steinization on nanoparticle characterization. Entries represent the numbers out of 600 data sets, designed to mimic results from scattering experiments intended for nanoparticle characterization [37], for which the "correct" configuration of nanoparticles was guessed based on the principle of minimizing L^2 distance. For example, entries in the "mean responses" rows pertain to minimizing L^2 distance between the scattering profiles estimated from a particular noisy data set and the actual scattering profiles for the "correct" configuration and three "incorrect" configurations of nanoparticles; whichever of these four L^2 distances is smallest determines the guess for the configuration of nanoparticles from which the particular noisy data set was generated. Since this was a simulation experiment, we knew which guesses were correct and could calculate correct classification rates. Scenarios 1 through 4 are as described in the caption to Table 2 above.

On the other hand, the former reductions tend to be greater than the latter reductions. This suggests that if we make our classifications probabilistic, by comparing the L^2 distances and assigning indices of plausibility to the various configurations, instead of merely identifying the most plausible configuration for a particular noisy data set, some further benefits of Steinization may manifest. For example, even if the correct classification rate is unchanged from 559/600 after Steinization is performed, perhaps the experimenter can go from being “80% confident” in the classifications to “90% confident” after Steinization. Of course, concepts such as “80% confident” and “90% confident” must be formalized, and this will be done later in our future research, but the point for now is that probabilistic classifications may be more definitive with Steinization than without. And, presumably, an experimenter would wish to have greater confidence in his or her inferences about nanoparticle configurations before using them to engineer nanostructured surfaces for efficient nano-TPV power generation. Thus, despite the mixed results in Tables 2 and 4 above, we have some viable avenues to pursue in our future research regarding the use of compound estimation in an inverse model for nanoparticle characterization geared toward efficient nano-TPV power generation. We eagerly look forward to pursuing these avenues, and we thank the ARO for its sponsorship of the phase of our work just completed.

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Appendix 1: Submissions or publications under ARO sponsorship

(a) Papers published in peer-reviewed journals: One publication, three submissions.

R. Charnigo, L. Feng, and C. Srinivasan. "Nonparametric and semiparametric compound estimation in multiple covariates," Submitted to *Biometrics* in June 2013.

R. Charnigo and C. Srinivasan. "A multivariate generalized C_p and surface estimation," Submitted to *Biostatistics* in September 2013.

S. Edalatpour and M. Francoeur, "The Thermal Discrete Dipole Approximation (T-DDA) for near-field radiative heat transfer simulations in three-dimensional arbitrary geometries," *Journal of Quantitative Spectroscopy and Radiative Transfer*, in press (DOI: 10.1016/j.jqsrt.2013.08.021), 2013.

M.R. Short, J.-M. Geffrin, R. Vaillon, H. Tortel, B. Lacroix, and M. Francoeur, "Evanescent wave scattering by particles on a surface: Validation of the discrete dipole approximation with surface interaction against microwave analog experiments," Submitted to *Journal of Quantitative Spectroscopy and Radiative Transfer* in October 2013.

(b) Papers published in non-peer-reviewed journals: None.

(c) i. Presentations at meetings, but not published in conference proceedings: Five conference presentations plus two invited presentations at academic institutions, delivered or scheduled.

R. Charnigo and C. Srinivasan, "A multivariate generalized C_p and surface estimation," University of Louisville, Louisville, KY, USA, November 15, 2013 (Invited presentation).

S. Edalatpour and M. Francoeur, "The Thermal Discrete Dipole Approximation (T-DDA) for numerical simulation of near-field thermal radiation," *ASME 2013 International Mechanical Engineering Congress & Exposition*, San Diego, CA, USA, November 15-21, 2013.

S. Edalatpour and M. Francoeur, "The Thermal Discrete Dipole Approximation (T-DDA) for near-field radiative heat transfer calculations," *2013 ASME Summer Heat Transfer Conference*, Minneapolis, MN, USA, July 14-19, 2013.

S. Edalatpour and M. Francoeur, “Numerical simulation of near-field thermal radiation using the Thermal Discrete Dipole Approximation,” *Electromagnetic and Light Scattering XIV*, Lille, France, July 17-21, 2013.

L. Feng, R. Charnigo, and C. Srinivasan. “James-Stein type compound estimation of multiple mean response functions and their derivatives,” *ENAR 2013 Spring Meeting*, Orlando, Florida, USA, March 10-13, 2013.

M. Francoeur, “Design of thermal metamaterials beyond the effective medium theory: Direct numerical simulation via the Thermal Discrete Dipole Approximation (T-DDA),” Institut National des Sciences Appliquées (INSA) de Lyon, Villeurbanne, France, June 13, 2013 (Invited presentation).

M.R. Short, H. Tortel, A. Litman, J.-M. Geffrin, R. Vaillon, R. Abdeddaim and M. Francoeur, “Evanescent wave scattering by particles on a surface: Comparison between the discrete dipole approximation with surface interaction and the finite element method,” *Electromagnetic and Light Scattering XIV*, Lille, France, July 17-21, 2013.

(c) ii. Non-peer-reviewed Conference Proceedings (other than abstracts): None.

(c) iii. Peer-reviewed Conference Proceedings (other than abstracts): None.

(d) Manuscripts: Five manuscripts in preparation to be submitted later in 2013 or 2014 (target journals listed below are tentative).

R. Charnigo, L. Feng, M. Francoeur, and C. Srinivasan, “Stein’s phenomenon and nanoparticle characterization,” *Journal of the Optical Society of America Series A*, to be submitted in 2014.

S. Edalatpour and M. Francoeur, “Near-field radiative heat transfer between complex-shaped objects and a surface,” *Physical Review Letters*, to be submitted later in 2013.

L. Feng, R. Charnigo, and C. Srinivasan. “Stein’s phenomenon in nonparametric regression,” *Journal of the Royal Statistical Society Series B*, to be submitted in 2014.

L. Feng, R. Charnigo, and C. Srinivasan. “James-Stein type compound estimation of multiple mean response functions and their derivatives,” *Journal of the American Statistical Association*, to be submitted in 2014.

R. Vaillon, B. Lacroix, J.-M. Geffrin, M. Francoeur, and R. Abdeddaim, "Far-field and near-field surface wave scattering microwave scanner," *Review of Scientific Instruments*, to be submitted later in 2013.

(e) Books: None.

(f) Honors and Awards: No honors or awards were made specifically for any of the papers written under this ARO sponsorship. However, Dr. Charnigo was promoted from associate professor (with tenure) to full professor (with tenure) at the University of Kentucky, effective July 1, 2013, in part due to internal and external recognition of this ARO sponsorship. Moreover, Dr. Francoeur received the NSF Career Award in July 2013 for demonstrating experimentally enhanced power generation in nanoscale-gap thermophotovoltaic power generators; he believes that this ARO sponsorship contributed to his acquisition of the NSF Award.

(g) Title of patents disclosed during the reporting period: None.

(h) Patents disclosed during the reporting period: None.

Appendix 2: Students and personnel supported

(a) Graduate students: Three graduate students partially supported.

Sheila Edalatpour, PhD candidate, Department of Mechanical Engineering, University of Utah (2011 – Present). Financial Support: 30% FTE for one semester (thus, approximately 11% of one year's effort).

Limin Feng, PhD, Department of Statistics, University of Kentucky (2008 – 2013). Financial Support: 100% FTE for a four-week interval between semesters (thus, approximately 8% of one year's effort). However, her total participation in ARO-sponsored research exceeded this amount of time because she also pursued the research in her dissertation, in partial fulfillment of the academic requirements for the PhD.

Mitchell R. Short, MS, Department of Mechanical Engineering, University of Utah (2011 – 2013). Financial Support: 100% FTE for one semester (thus, approximately 38% of one year's effort).

(b) Post doctorates: None.

(c) Faculty

Richard Charnigo, Professor, Departments of Statistics and Biostatistics, University of Kentucky. Support: 1.47 months' salary (thus, approximately 12% of one year's effort).

Mathieu Francoeur, Assistant Professor, Department of Mechanical Engineering, University of Utah. Support: 0.50 months' salary (thus, approximately 4% of one year's effort).

Cidambi Srinivasan, Professor, Department of Statistics, University of Kentucky. Support: 1.47 months' salary (thus, approximately 12% of one year's effort).

(d) Undergraduate students: None.

(e) Graduating undergraduate metrics: Not applicable.

(f) Master degrees awarded: One.

Mitchell R. Short, MS, Department of Mechanical Engineering, University of Utah, 2011-2013. Thesis title: The discrete dipole approximation with surface interaction for evanescent wave-based characterization of nanostructures on a surface with validation against experimental results.

(g) PhDs awarded: One.

Limin Feng, PhD, Department of Statistics, University of Kentucky, 2008-2013. Dissertation title: James-Stein type compound estimation of multiple mean response functions and their derivatives.

(h) Other research staff: None.

Appendix 3: Technology transfer

There are no inventions or patents associated with this ARO sponsorship. However, the statistical methods proposed in "Nonparametric and semiparametric compound estimation in multiple covariates" and "A multivariate generalized C_p and surface estimation" have been implemented in the R computing environment. These implementations will be made freely available to anyone, upon request to Dr. Charnigo, once the corresponding manuscripts have been published in peer-review journals.

Appendix 4: Copies of technical reports

The manuscript "Stein's phenomenon and nanoparticle characterization" already exists in technical report form and has been uploaded to the ARO reporting website along with this final project report. The manuscript will be improved and submitted to the *Journal of the Optical Society of America Series A*, or a similar peer-review journal, in 2014. We have also uploaded manuscripts that have already been submitted to but have not yet been accepted by peer-review journals, as well as conference or presentation abstracts, the MS thesis of Mitchell Short, and the PhD dissertation of Limin Feng.